EFFECT OF PRESENCE OF DOUBLE NOTCH ALONG WITH VARIOUS GEOMETRY ON TENSILE AND COMPRESSION BEHAVIOUR OF PURE COPPER USING MOLECULAR DYNAMICS SIMULATION

A thesis submitted in partial fulfillment of the requirements for the degree of Bachelor of

Technology in Metallurgical and Materials Engineering

By

Chinmaya Kumar Mallick (110MM0363)

Under the supervision

of

Prof. Krishna Dutta

Department of Metallurgical and Materials Engineering National

Institute of Technology, Rourkela

2014

DEPARTMENT OF METALLURGICAL AND MATERIALS ENGINEERING

NATIONAL INSTITUTE OF TECHNOLOGY , ROURKELA ,

ODISSA , PIN-769008 , INDIA

CERTIFICATE

This is to certify that the thesis entitled "**EFFECT OF PRESENCE OF DOUBLE NOTCH ALONG WITH VARIOUS GEOMETRY ON MECHANICAL PROPERTIES OF PURE Cu USING MOLICULAR DYNAMICS SIMULATION"**, submitted to National Institute of Technology, Rourkela by **Chinmaya Kumar Mallick(110MM0363)** in partial fulfillment of the requirements for the award of the degree of **BACHELOR OF TECHNOLOGY** in **Metallurgical and Materials Engineering** is an authentic work carried out by them under my supervision and guidance. The matter embodied in the thesis has not been submitted to any other University/ Institute for the award of any degree or diploma.

Prof. Krishna Dutta

Department of Metallurgical and Materials

Engineering

National Institute of Technology Rourkela

ACKNOWLEDGEMENTS

This project wouldn't have been possible without the help, support, and cooperation of many peoples. At the beginning, I would like to express my sincere thankfulness to my supervisor Prof. Krishna Dutta for his indispensable guidance and support at all times and his guidance throughout the duration of the project. I also avail this opportunity to extend my indebtedness to Prof. NatrajYedla for his valuable guidance, constant encouragement and kind help and advice at various stages during the execution of this work. Their encouragement and comments kept our effort alive, and helped me to establish the overall direction of the project.

I would also like to express my gratitude to Prof. S.C.Mishra , Head of the Department, Metallurgical and Materials Engineering for allowing me access to the laboratory facilities in the department.

My sincere thanks to family and friends who have provided me with inspirational words, a welcome ear, new ideas, and their invaluable time.

Chinmaya Kumar Mallick
Roll no: 110MM0363

Department of Metallurgical and Materials Engineering,
National Institute Of Technology, Rourkela
Rourkela-769008

ABSTRACT

The aim of this experiment is to study the effect of double notch of various geometries on the tensile and compression behaviors of nanoscale copper at various temperatures through simulations based on molecular dynamics. To do this, first simulation boxes have been created comprising of Double cylindrical, Double square and Double v-notches. Simulations for tensile and compression deformations have been done for all un-notched and Double notched specimens at different temperatures (viz. 100 K, 300 K and 500 K). The results indicate that yield and tensile strength values decreases with increase in temperature for all notched and double un-notched simulation boxes. Strength values increase with introduction of notches of all geometries as compared to the double un-notched ones, at all temperatures .In contrast to the tensile strength, it is found that the compression strength of notched specimen decreases with introduction of notches at a particular temperature .The variation in strength is attributed to the formation of stress triaxiality around the tip of the notch and plastic constraint factor. The square notch is the highest contributor to increase the tensile strength. Overall, it can be stated that molecular dynamic simulation can be effectively used to study the deformation behaviour of notched specimens.

CONTENTS

- Input file for obtaining 3D crystal lattice of Double V-notched sample using lammps

3.5. Tensile test

- Input file for tensile testing using LAMMPS
- The Ductile fracture in nano-scaled copper through tensile simulation code

3.6. Compression test

- Input file for compression testing using LAMMPS
- The Brittle fracture in nano-scaled copper through compression simulation code

4. RESULTS AND DISCUSSION

4.1. Tensile properties

- Effect of temperature on tensile behaviour
- Effect of notch design on tensile behaviour

4.2. Compression properties

- Effect of notch design on compression behaviour

5. CONCLUSIONS AND SCOPE OF FUTURE WORK

6. REFERENCE

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

OUTLINE

- BACKGROUND OF RESEARCH
- OBJECTIVES OF THE PROJECT
- SUMMERY

1.1. Background of research:

We known that for using a material for any type of engineering application, we needs to investigate the mechanical properties of the that material which is include tensile and compression deformation behaviour, its stiffness, hardness etc. Usually tensile behaviour of a ductile material is studied using a dog bone shape of specimen as per ASTM standard E8M . In more detailed, it can be stated that the central part of this type of a specimen is smooth. One can generally predict that the mechanical properties of a specimen may vary based on the conditions of the surface of the specimen. Ductility measurements of standard smooth tensile specimens don't always reveal environmental or metallurgical changes that lead to reduced local ductility. On apply loading, the stress distribution of a specimen varies in case of presence of a discontinuity on the surface of it. This kind of stress distribution may be considered as tri axial state of stress. The inclination for reduced ductility in presence of a tri-axial stress field and steep stress gradients is called as notch sensitivity. In practical case, a component/material always have some irregularities like pores, cracks etc. on or below the surface. Therefore it is always needed to study the mechanical behaviour of the material when irregularities are there. This will help to predict the mechanical behaviour in actual service condition.

There are various shape of notches used during a simulation. Various types of notch geometry can alter the mechanical behaviour to the specimen. But in lab experiment we generally use Double V-notched specimen. But in actual practice notch may be of different geometry like angular, square, cylindrical, spherical, conical etc. There are irregularities present in different types of notch geometries.

Computer based molecular dynamics (MD) simulation is now-a-days potentially utilized to determine different material behaviours. Computer simulations act as a channel between microscopic length and time scales and the macroscopic world of the laboratory. It provides information related to the interactions between atoms, and exactly predicts the mechanical properties. The predictions and observation can be made as precise and accurate as we like, subject to the limitations done by our computer's ability .Using molecular dynamics (MD) simulation, fracture mechanisms of nanoscale pure iron under static and symmetric cyclic loading conditions have been performed by Inoue et al .Li and his co-workers investigated the cyclic stress/strain evolutions for tensile strength prediction through simulation studies; it was found that the determination of tensile strength depends not only on the specimen models, but also on the accurate evaluations of the cyclic elasto-plastic stress/strain responses . The tensile and compression behaviour of nano-scale copper along with vacancies at different temperatures has been studied using MD simulation by Chang. Chang and Fang investigated the influence of tensile and compression behaviour of nanoscale copper through MD simulation. The mechanical properties of nano-structured copper have been of important interest to researchers due to the development of electronic industries. Most of the existing investigations are based on experimental results and findings. Reports are also available based on simulation of tensile and

compression behaviour through simulated models. As molecular dynamics (MD) simulation encounters studying the behaviour of 99.99% pure material, in this investigation tensile and compression behaviour of pure copper is studied to understand the effects of notch geometry in it.

1.2. Objectives

The main goal to fulfil these can be briefly stated as:

(I)To find tensile and compression behaviour of nano-scale copper at different temperatures:-

This part consists of

(a) Generating plots for tensile stress vs. strain curves of nano-scale copper at different temperatures for both notched and un-notched specimen.

(b) Study variation in the tensile and compression strength, yield strength of nano-scale copper at different temperatures.

(c)Study variation in % total elongation and % uniform elongation at variation of temperature.

(2)To find tensile and compression behaviour of nano-scale copper at different notch geometries:-

(a) Generating plots for tensile stress vs. strain curves of nanoscale copper at different notch geometries.

(b) Study variation in the tensile and compressive strength of nanoscale copper at different notch geometries at a particular temperature.

1.3. Summary:

The thesis has five chapters. There is briefing of the significance of the problem and relates research behind this investigation in **Chapter-1**. Some relevant literature background related to the current investigation of tensile and compression behaviour and molecular dynamics simulation has been presented in **Chapter-2**. **Chapter-3** consists of simulation parameters to perform simulation studies on nano-scale copper along with the description of the simulation procedure regarding tensile and compression behaviour behind these simulations. **Chapter-4** consists the results and discussion related to the above stated objectives. **Chapter-5** is an overview of the conclusions derived from this study which has been analyzed briefly with few directions for future work related to this section. A comparison has also been made with the results obtained from this investigation with those of previous investigations. All references cited throughout the work have been compiled at the end of **Chapter-5**.

CHAPTER 2

LITERATURE SURVEY

OUTLINE

- Introduction
    - Parameters related to stress vs strain curve
    - Effects Notches
- Some previous investigation related to this study
- Molecular dynamics simulation
- Advantages of using molecular dynamics simulation
- Review of the current problem

2 .1 INTRODUCTION:

The magnitude and shape of stress-strain curve of a material depends on its, heat treatment strain rate, composition, temperature etc.

2.1.1 PARAMETERS RELATED TO STRESS VS STRAIN CURVE:

ULTIMATE TENSILE STRENGTH

The ultimate tensile strength (UTS) is calculated by dividing the maximum load by the cross sectional area of specimen.

$S_u = P_{max} / \underline{A_o}$

The UTS is calculated from results of a tension test. For ductile material UTS is termed as measure of the maximum load which a metal can withstand under very restrictive condition of uniaxial loading .For many years it was used to define the strength of materials on tensile strength. But in recent times it is used of basing the static design of ductile metals on the yield strength. However because of long duration of using tensile strength to determine the strength of the materials, it has become a familiar property and identification of the materials.

MEASURE OF YIELDING

The stress at which plastic deformation or yielding is observed depends on the sensitivity of strain measurements. For most materials there is a gradual transition from elastic to plastic behaviour, the particular point at which plastic deformation begins is hard to tell. Various criteria for the initiation of yielding are used depending on the sensitivity of the strain measurements. Fig-2.1 gives the basic idea of stress vs strain curve

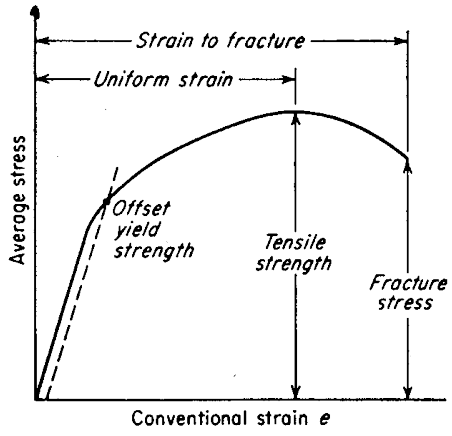


Fig-2.a. Stress vs strain curve

Elastic limit is the maximum stress the material can withstand without any measurable strain remaining on the complete release of load. With increasing sensitivity of strain measurement, the elastic limit is reduced

until it equals to true elastic limit. Determination of elastic limit requires too long loading-unloading test procedure. The yield strength is the stress required to produce a small amount of plastic deformation.

So=P (strain offset=0.002)/Ao

From the stress-strain curve we can determine the % uniform elongation and % total elongation.% uniform elongation is the point at the UTS at which necking starts. Up to this point the elongation will be uniform. After necking there come voids in the specimen. So the elongation will not be uniform anymore. At the fracture point the total strain will be % total elongation.

MODULUS OF ELASTICITY

It is the slope of the linear portion of the stress-strain curve. It is a measure of stiffness of the material. The MODULUS OF ELASTICITY is determined from the binding force of the atoms. These forces can't be changed without changing the nature of material. So it is the most structure insensitive property of the material. With increasing temperature the UTS and hence the Young's modulus of the material decreases.

2.1.2 EFFECT OF NOTCHES:

The changes produced by the notch geometries have significant consequences in fracture process. With the introduce of notch it creates a local stress peak at the root of the notch .Plastic flow begins here when local stress reaches yield strength of the material. The plastic flow limits the peak stress to yield stress of the material. The main effect of the notch is to create stress tri-axiality at the notch.

The elastic stress distribution in a notched thin plate is shown in fig 2.2.1. In this case two directional stresses are developed at the notch. Transverse elastic stress σ_x and longitudinal stress σ_y is generated. But for thick specimen as fig 2.2.2. Three components of stresses are generated at the notch tip. The distribution of σ_z with z at the notch root (x=0) is shown in fig-2.2.3. The values of σ_y and σ_x are nearly independent of z. Fig 2.2.2 shows that stressing a thick specimen provides stress triaxiality at the notch tip. As a consequence of stress triaxiality at the notch the yield stress will be more as compared to uniaxial yield stress because it is more difficult to spread yielded zone in case of stress triaxiality. The ratio of notched to unnotched flow stress is called plastic constraint factor. Orwan has shown this value cannot exceed 2.57. Thus this triaxial stress of a notch results in notch strengthening in a ductile metal but in case of brittle material this value exceed before the material undergoes plastic yielding.[2]

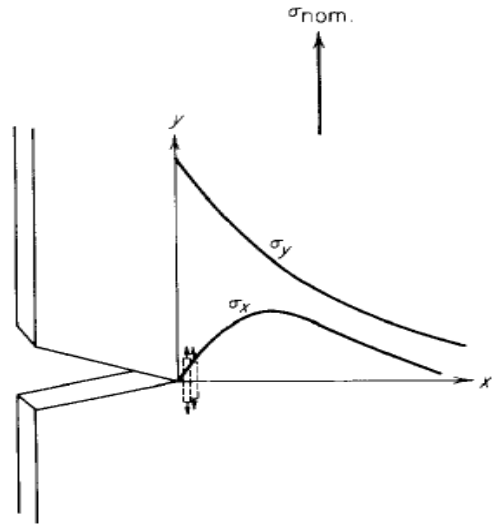


Fig.-2.b.i. Elastic stresses under a notch in a thin plate

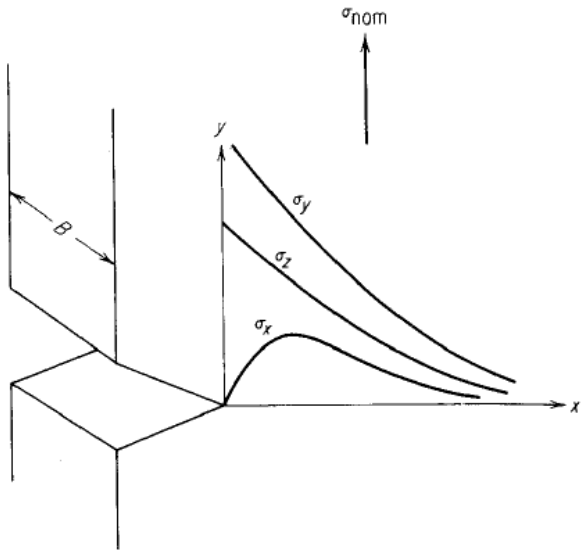


Fig.-2.b.ii Elastic stresses under a notch in a thick plate

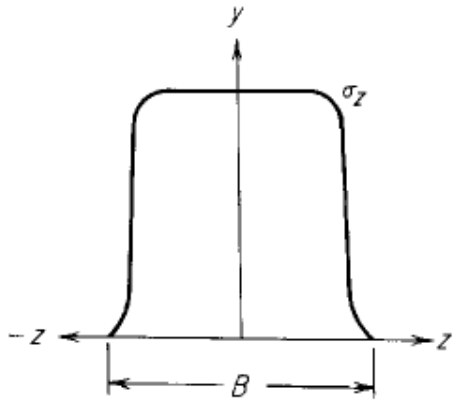


Fig-2.b.iii. Distribution of σ_z with z at x=0

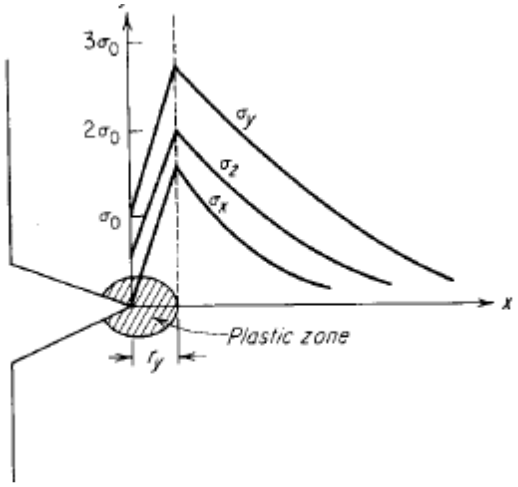


Fig-2.b.iv. Distribution of stresses during local yielding

The tendency for reduced ductility in presence of a triaxial stress field is called notch sensitivity. With the introduction of notch there comes a plastic constraint factor. Because of this plastic constraint factor tensile strength will be more than an unnotched specimen. The common way to detect notch brittleness or high notch sensitivity is by calculating notch strength ratio (NSR).

NSR=Snet (for notched specimen)

Su (tensile strength for unnotched specimen)

If NSR<1, then material is notch brittle. There is also reduction of area at the notch.

2.2 SOME PREVIOUS INVESTIGATION RELATED TO THIS STUDY:

Over the past ten years, the study on the mechanical properties of nano-scaled materials by using atomistic simulation has been of important interest to researchers due to nano-technological development [8–10]. For example, Miyazaki and Shiozaki [3] were calculated the elastic constant and thermal expansion coefficient of Fe. Aya and Nakayama [11] investigated the influence of environmental temperature on the yield stress of polymers. For a material the material stiffness is one of the important properties . Miller and Shenoy [11] studied the bending stiffness properties of nanosized structural Al and Si. Since the development of the electronic industry, copper has been one of the significant materials in the field, used in, for example, electrical interconnects [13]. Many studies have look at the material properties of copper. Heino et al. [14]

investigated the mechanical properties of copper, including the elastic constant and the behavior of crack propagation at room temperature .Schiotz et al. [15] studied the effects of strain rate and porosity on the mechanical deformation of copper at various temperatures. Recently, Kang and Hwang [16] investigated mechanical deformations of copper nanowire.

Earlier researchers have studied about the behaviour of nano-scale copper using MD simulation. But Chang has studied the mechanical behaviour of nano-scale copper where vacancies are present inside the box using MD simulation as fig-2.2. The behaviour will change as compared to the normal box dimension.

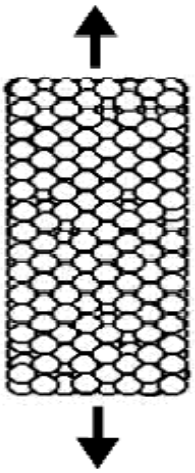


Fig-2.c. Configuration of nano-scale copper with vacancies for the tensile test[6]

He has studied the tensile behaviour for various amount of vacancies at a particular temperature and the effect of tensile behaviour on temperature as shown in fig-2.3, 2.4. From the investigation he conclude that with increase in vacancies of nano-scale copper the UTS decreases considerably. He also concluded that the UTS of nano-scale copper decreases with increase in temperature. His investigation may help us for our study related to tensile and compression behaviour of nano-scale copper using MD simulation.

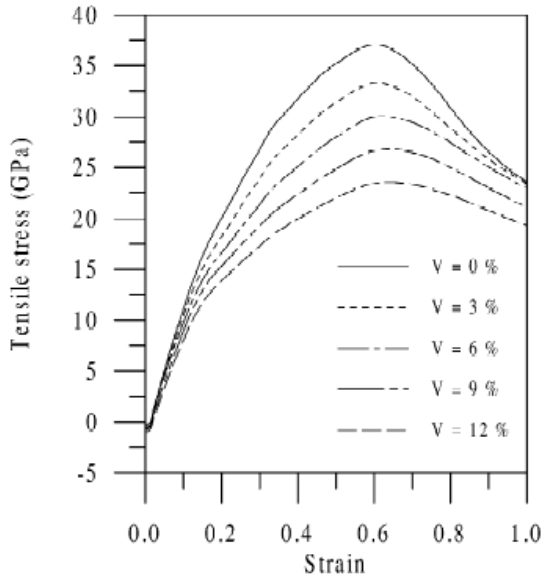


Fig. 2.d. Relationship between tensile stress and strain for nanoscale copper with various vacancies at *T*5300 K

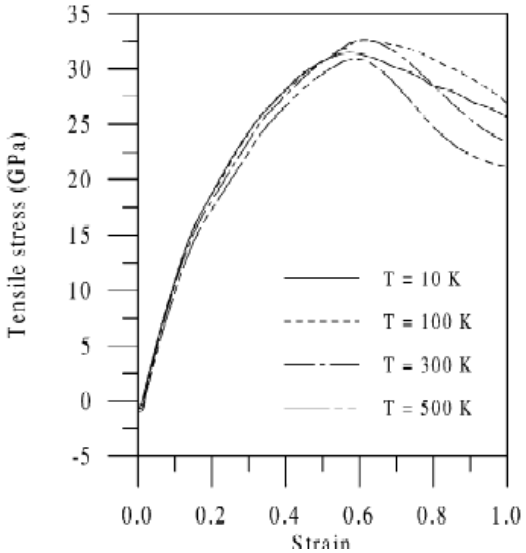


Fig. 2.e. Relationship between tensile stress and strain for nanoscale copper with *V*56% at various temperatures.

2.3Molecular dynamics simulation:

Molecular dynamics (MD) simulation is a computer based simulation of the movements of atoms and molecules which are allowed to interact with each other for a period of time. Generally, the trajectories of atoms and molecules are determined by solving the Newton's equations of motion for a system of interacting particles, where forces among particles are defined by force fields of molecular mechanics. These simulations can be used to determine macroscopic thermodynamic properties of the system. MD simulation is also known as statistical mechanics by

numbers" and "Laplace's vision of Newtonian mechanics" as it predicts the future by animating the forces of nature and providing a view into motion of molecules on an atomic scale. A molecular dynamics simulation requires a description of the particles in the simulation which will interact. The advantage of MD is that it gives an idea of dynamical properties of the system: transport coefficients, time-dependent responses to perturbations, rheological properties and spectra. Potentials may be defined at many levels of physical accuracy; those most commonly used in chemistry are based on molecular mechanics and personify a classical treatment of particle-particle interactions that can generate structural and conformational changes but usually cannot produce chemical reactions.

2.4 Advantages of using Molecular Dynamics Simulation:

- For the investigators conducting tensile and compression tests at high temperature really a challenge and needs long duration of time. Hence many molecular simulation studies have come into picture to predict the tensile and compression behaviour of materials at various temperatures.
- Using molecular dynamics simulation, 100% pure copper can be obtained theoretically but it is practically impossible.
- Moreover, testing can be carried out at low temperature, room temperature and elevated temperatures at the same time, facilities for which are not available in my labs.
- To create perfect notch of different geometries practically is difficult and time taking. Using MD simulation we can ignore these difficulties.

In this report an attempt has been made to gain some knowledge on tensile and compression behaviour of materials through MD simulations.

2.5 Review of the current problem:

There are numerous investigations related to tensile and compression behaviour of materials under different temperature and stress applied.

Most of these investigations mostly verify the effect of temperature on the tensile and compression property of nanoscale copper and how the presence of different types of notch geometry differs from the un-notched condition.

This investigation, in brief, attempts to understand:

(i) Tensile behaviour of the investigated material i.e. nano-scale copper at various temperatures and different types of notch geometry.

(ii) The % elongation and tensile strength at various temperatures and notch geometry in nano-scale copper.

CHAPTER 3

MOLECULAR DYNAMICS SIMULATION USING LAMMPS

OUTLINE

- Introduction
- Simulation procedure
- Simulation parameters
- Sample configuration
    - Input file for obtaining 3D crystal lattice of un-notched sample using lammps
    - Input file for obtaining 3D crystal lattice of Double square-notched sample using lammps
    - Input file for obtaining 3D crystal lattice of Double cylindrical-notched sample using lammps
    - Input file for obtaining 3D crystal lattice of Double V-notched sample using lammps

- Tensile test of all samples
    - Input file for tensile testing using LAMMPS
    - The Ductile fracture in nano-scaled copper through tensile simulation code

- Compression test of all samples
    - Input file for compression testing using LAMMPS
    - The Brittle fracture in nano-scaled copper through compression simulation code

3 MOLECULAR DYNAMICS (MD) SIMULATION USING LAMMPS:

3.1 INTRODUCTION:

In this experiment, Molecular Dynamics (MD) simulation of nano-scale copper has been tested LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). LAMMPS is a molecular dynamics simulation code designed to run efficiently on parallel computers. It is an open-source code that models an ensemble of particles in a liquid, solid, or gaseous state. It can model atomic, polymeric, metallic, granular, and coarse-grained systems using a variety of force fields and boundary conditions.

LAMMPS integrates Newton's equations of motion for collections of molecules, atoms, or macroscopic particles which interact by short- or long-range forces with a variety of boundary conditions. For computational efficiency, LAMMPS uses neighbor lists
(Optimization of systems with particles which are repulsive at short distances, so that local Density of particles will never become too large) to keep track of nearby particles. On parallel Machines, to partition the simulation domain into small 3d sub-domains, LAMMPS uses spatial decomposition techniques.

A LAMMPS input script includes 4 parts such as:

1. Code Initialization
2. Defining Atoms
3. Settings
4. Running a simulation

LAMMPS runs commands from an input script (.txt file), reading one line at a time. When the input script ends it exits automatically. Every command causes LAMMPS to perform an action; it can read in a file, set an internal variable, or run a simulation. Generally, in an input script the ordering of commands is insignificant.

However below mentioned points should be taken care of:

(1) LAMMPS reads one line at a time from the input script and then each and every command takes effect immediately after when it is read, not after the complete text file is read.

(2) A few commands are valid only when they follow other commands. A group Command can be used only after the atoms were defined.

(3) Sometimes a command Y may use values set by command X. This means command Y must follow command of X in the input data if it needs to have the necessary effect.

3.2 Simulation procedure:

In my simulations I used EAM FS (Finnis-Sinclair) potential developed by Mendelev et al [23]
And it is a valid potential. In the EAM, the total energy of an *N*- atom system is represented in the Following equation:

$$E_{\text{tot}} = \sum_i F_i(\rho_i) + \frac{1}{2} \sum_{\substack{i,\ j \\ i \neq j}} \varphi_{i,\ j}(r_{i,\ j})$$

Where *i, j* (*ri, j*) is a short range pair potential between atom i and *j* with the separation distance *i j r , , ( ) ii F* □□is the embedding energy of atom *i* with the electron density *i*□□due to all its neighbors is expressed below:

$$\rho_i = \sum_{j \neq i} f_j(r_{ij})$$

In Finnis/Sinclair stated the total energy of an atom can be described by the following equation:

$$E_i = F_\alpha\left(\sum_{j \neq i} \rho_{\alpha,\beta}(r_{i,j})\right) + \frac{1}{2}\sum_{j \neq i} \varphi_{\alpha,\beta}(r_{i,j})$$

where □□the electron density is a functional specific to the atomic types of both atoms *i* and *j* so that different elements can contribute differently to the total electron density at an atomic site depending on the identity of the element at that atomic site and alpha and beta are the element types of atom *i* and *j*. The initial amorphous structures for simulation were obtained using NPT ensemble with zero applied pressure. Time step is equal to 0.002 ps. Equations of motion are numerically integrated using velocity-Verlet algorithm.

3.3. Simulation Parameters:

LAMMPS requires as input a list of initial atom coordinates and types, molecular topology information, and force-field coefficients assigned to all atoms and bonds. It has potentials for soft materials viz. biomolecules, polymers; solid-state materials viz. metals, semiconductors and coarse-grained or microscopic systems .VMD is a simple and fast visualizer provided with the LAMMPS package which

creates xyz projection views of atomic coordinates and animates them. Through VMD we can visualize the changes taking place step by step in the simulation.

While writing the simulation input file code, variables like potential file, lattice parameters, maximum and minimum stress, temperature, number of cycles and number of iterations are changed. These parameters govern the simulation conditions and environment. For atomic systems LAMMPS provides a create atoms command which places atoms on solid-state lattices (fcc , bcc, user-defined, etc.). Assigning small numbers of force field coefficients can be done via the pair coeff, bond coeff, angle coeff, etc commands.

Simulation box size, time step and total duration must be adjusted such that the calculation can finish within a reasonable time period. However, the simulations should be made as long as it can be so as to match the time scales of the natural processes being studied. In other words, to make statistically valid conclusions, the time span of the simulation should match the kinetics of the natural process. The time step should be small enough so as to avoid discretization errors (i.e.it must be smaller than the frequency of fastest vibrations of the system). The simulation box size must be large enough to avoid boundary condition artifacts. Boundary conditions are often treated by choosing fixed values at the edges (which may cause artifacts), or by employing periodic boundary conditions in which one side of the simulation loops back to the opposite side, imitating a bulk phase.

NVE (Micro-canonical ensemble): In NVE ensemble, the system undergoes an adiabatic Process and is isolated from changes in moles (N), volume (V) and energy (E).

NVT (Canonical ensemble): In NVT, also sometimes called as constant temperature molecular dynamics (CTMD), moles (N), volume (V) and temperature (T) are conserved and the energy of endothermic and exothermic processes is exchanged with a thermostat.

NPT (Isothermal–isobaric) ensemble: In NPT ensemble, moles (N), pressure (P) and Temperature (T) are conserved. A barostat is also needed along with a thermostat. It corresponds to laboratory conditions with a flask open to ambient temperature and pressure

3.4. Sample Configuration:

The initial configuration of four different samples for various molecular dynamics simulations is shown in Fig. 1,Fig. 2, Fig.3 and Fig. 4. Both tensile and compression simulations were performed using this type of sample configuration. The assembly contains three regions; grip region at the opposite ends which is composed of immobile atoms and tension/tension-compression region which include the mobile atoms. Tensile and Compression loading were carried out in the both x,y-direction, as indicated in Fig. 3.0. The periodic boundary condition was imposed on the x and z axis and the material was free to be strained in the y-direction only.

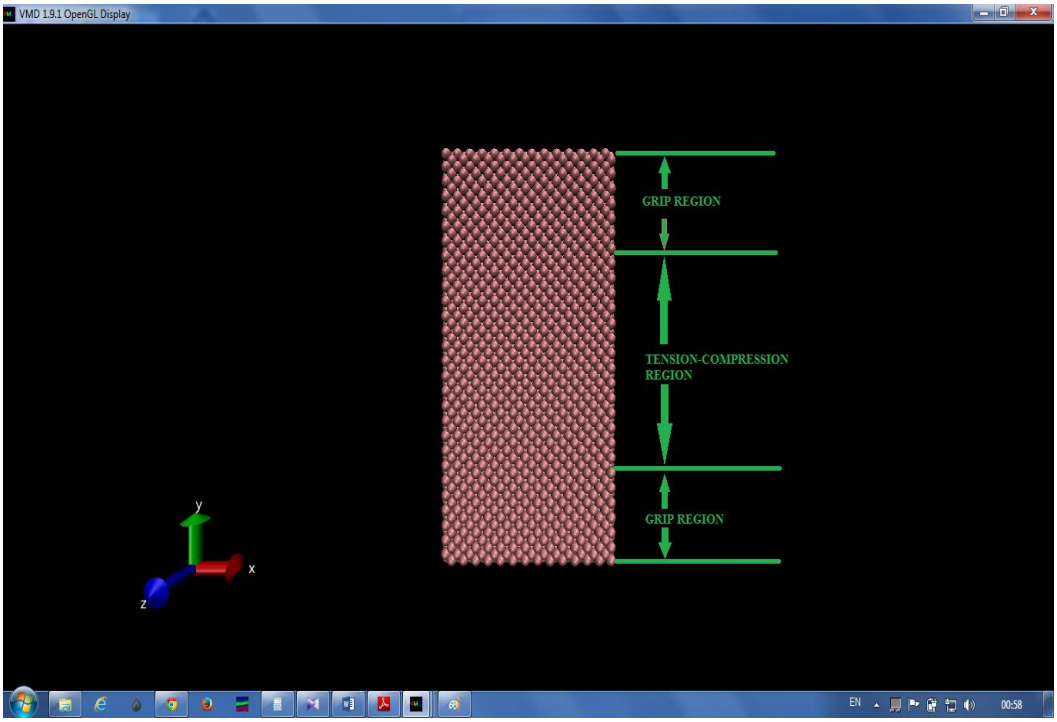
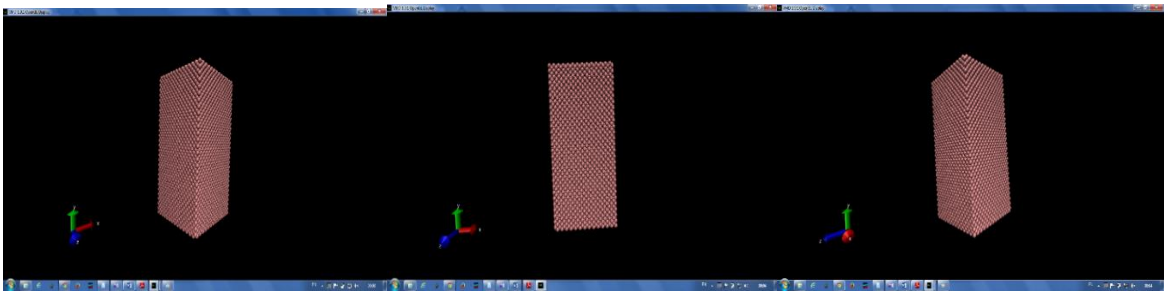
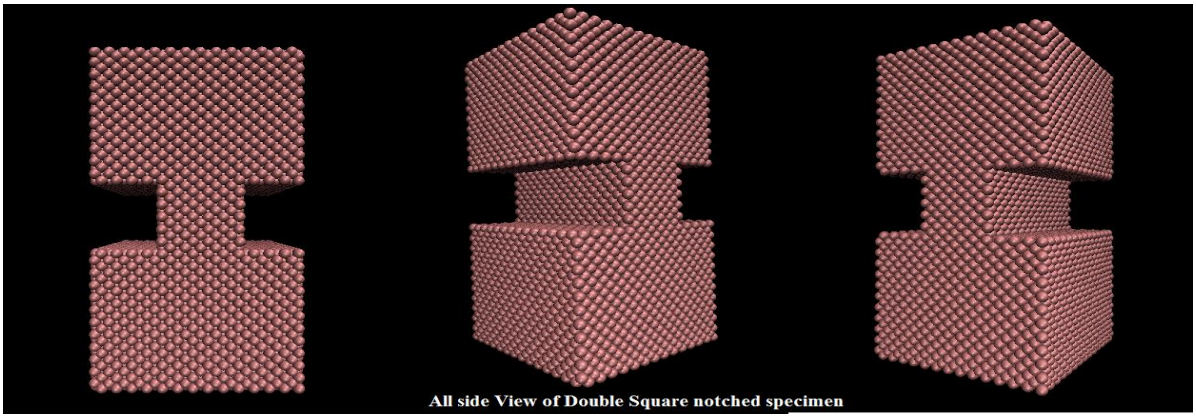


Fig.3.a.i: VMD snapshot of the Cu sample undergoing simulation.



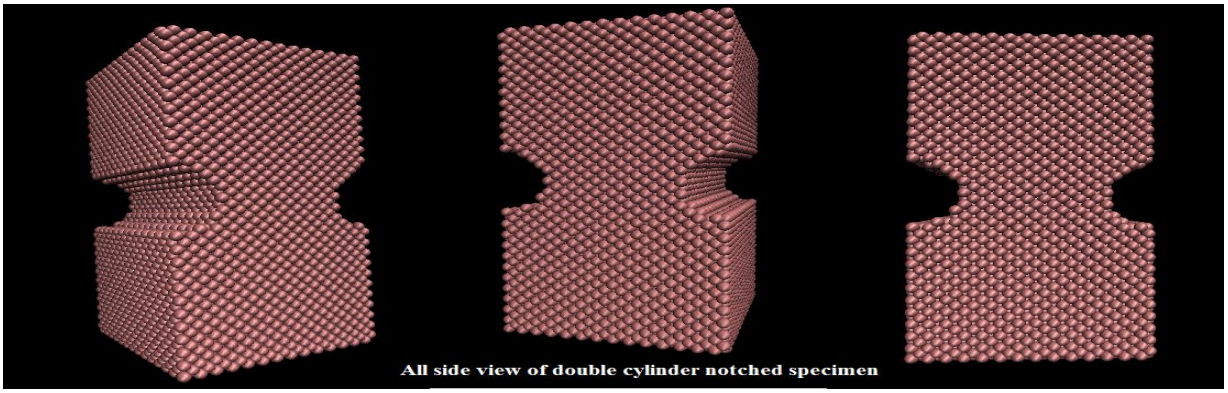
(Left side view) (Front view) (Right side view)

Fig. 3.a.ii: Different sectional view of Un-notched Sample:



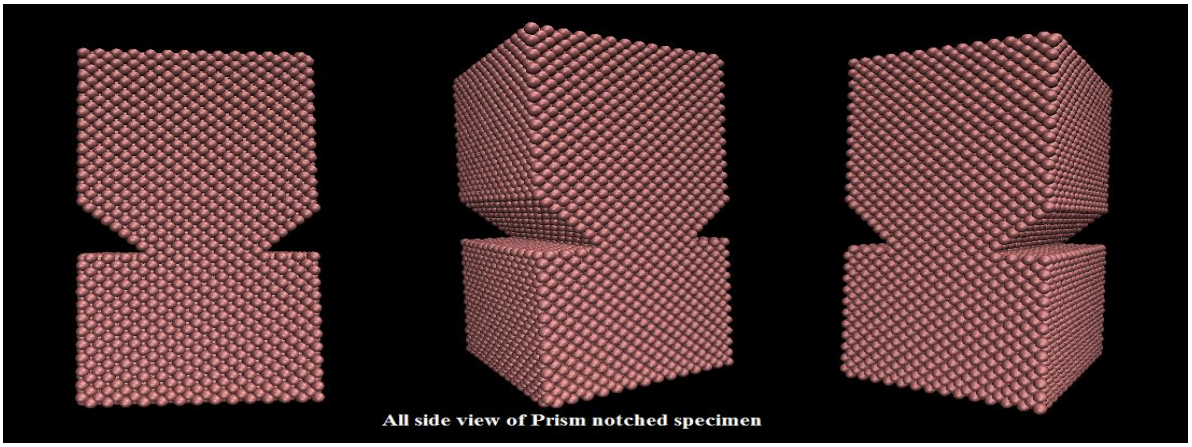
(Front view) (Left side view) (Right side view)

Fig. 3.a.iii: Different sectional view of Double square-notched Sample:



(Left side view) (Right side view) (Front view)

Fig. 3.a.iv: Different sectional view of Double cylindrical-notched Sample:



(Front view) (Left side view) (Right side view)

Fig. 3.a.v: Different sectional view of Double V-notched Sample:

SI. No.	Sample type	Box Dimension	Total number of Atoms
1.	Un-Notched	50 x 100 x 50	21952
2.	Square-Notched	50 x 100 x 50	20720
3.	Cylinder-Notched	50 x 100 x 50	20566
4.	V-Notched	50 x 100 x 50	21056

Table 3.4.1: Size and Dimensions of Sample with different notch geometry Undergoing Simulation

3.4.1. Input file for obtaining equilibrated 3D-crystal lattice of Un-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…** **determines units of all quantities used in the input file**
echoboth **…** **echoes each input script command to both log file and screen**
atom_style atomic
dimension 3
boundary p pp**…** **periodic boundary condition**
region box block 0 50 0 100 0 50 units box **defines a geometric region of space**
create_box 1 box**.....** **creates a simulation box in the specified region**

lattice fcc 3.61**……..** **lattice type and lattice parameter**
region cu block 0 50 0 100 0 50 units box
create_atoms 1 region cu units box**…** **creates copper atoms in the simulation box**

timestep 0.002**……** **sets the timestep for subsequent simulations**
pair_styleeam/alloy
pair_coeff * * Cu_zhou.eam.alloy Cu**……** **specifies the potential file used**

 # Energy Minimization
#minimize 1.0e-7 1.0e-8 1000 1000
thermo 100 **computes and prints thermodynamic**
thermo_style custom step temp vol press etotal **specifies content of thermodynamic**
data to be printed in screen &

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

…..dumps a snapshot of atom quantities every 10 time steps

to the specified file

dump_modify 1 scale no**…modifies parameters of previously defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian **…sets the velocity of a group of atoms**

#fixes

#fix 1 all npt temp 100 100 0.1 iso 0 0 0.1**temp and pressure conserved**

run 1000**… program is run for 1000 iterations**

unfix 1 **… deletes the previously defined fix 1**

3.4.2. Input file for obtaining equilibrated 3D-crystal lattice of Double Square-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **… determines units of all quantities used in the input file**

echoboth **… echoes each input script command to both log file and screen**

atom_style atomic

dimension 3

boundary p pp**…periodic boundary condition**

region box block 0 50 0 100 0 50 units box **defines a geometric region of space**

create_box 1 box**.....creates a simulation box in the specified region**

lattice fcc 3.61**……..lattice type and lattice parameter**

region cu block 0 50 0 100 0 50 units box

create_atoms 1 region cu units box**… creates copper atoms in the simulation box**

region cu1 block 35 50 40 60 0 50 units box**defines a geometric region of Square-notch**

group crystal region cu1

delete_atoms group crystal**…** **creates one side square-notch in the simulation box**

region cu2 block 0 15 40 60 0 50 units box

group crystal region cu2

delete_atoms group crystal**…** **creates another side square-notch in the simulation box**

timestep 0.002**……** **sets the timestep for subsequent simulations**

pair_styleeam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu**……** **specifies the potential file used**

 # Energy Minimization

#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100 **computes and prints thermodynamic**

thermo_style custom step temp vol press etotal **specifies content of thermodynamic**

data to be printed in screen &

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

..… **dumps a snapshot of atom quantities every 10 time steps**

to the specified file

dump_modify 1 scale no**…** **modifies parameters of previously defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… **closes the current log file, opens a new log file, and begins logging information to it**

velocity all create 300 873847 rot yes mom yes distGaussian **…** **sets the velocity of a group**

of atoms

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1 **temp and pressure conserved**

run 1000**…** **program is run for 1000 iterations**

unfix 1 **…** **deletes the previously defined fix 1**

3.4.3. Input file for obtaining equilibrated 3D-crystal lattice of Cylinder-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **…** **determines units of all quantities used in the input file**
echoboth **…** **echoes each input script command to both log file and screen**
atom_style atomic
dimension 3
boundary p pp**…** **periodic boundary condition**
region box block 0 50 0 100 0 50 units box **defines a geometric region of space**
create_box 1 box**.....** **creates a simulation box in the specified region**

lattice fcc 3.61**……..** **lattice type and lattice parameter**
regioncu block 0 50 0 100 0 50 units box
create_atoms1 region cu units box**…** **creates copper atoms in the simulation box**

region cu1 cylinder x 50 40 10 0 50 units box **defines a geometric region of Cylinder-notch**
group crystal region cu1
delete_atoms group crystal**…** **creates square-notch in the simulation box**

timestep 0.002**……** **sets the timestep for subsequent simulations**
pair_styleeam/alloy
pair_coeff * * Cu_zhou.eam.alloy Cu**……** **specifies the potential file used**

 # Energy Minimization
#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100 **computes and prints thermodynamic**
thermo_style custom step temp vol press etotal **specifies content of thermodynamic**
data to be printed in screen &

computemyRDF all rdf 1000
fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj
..… **dumps a snapshot of atom quantities every 10 time steps**
to the specified file
dump_modify 1 scale no**…** **modifies parameters of previously defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… closes the current log file, opens a new log file, and begins logging information to it

velocity all create 300 873847 rot yes mom yes distGaussian **…sets the velocity of a group of atoms**

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1**temp and pressure conserved**

run 1000**… program is run for 1000 iterations**

unfix 1 **…deletes the previously defined fix 1**

3.4.4. Input file for obtaining equilibrated 3D-crystal lattice of V-notched sample using LAMMPS:

 # This program is for obtaining 3d-crystal lattice

units metal **… determines units of all quantities used in the input file**

echoboth **… echoes each input script command to both log file and screen**

atom_style atomic

dimension 3

boundary p pp**…periodic boundary condition**

region box block 0 50 0 100 0 50 units box **defines a geometric region of space**

create_box 1 box**.....creates a simulation box in the specified region**

lattice fcc 3.61**……..lattice type and lattice parameter**

region cu block 0 50 0 100 0 50 units box

create_atoms 1 region cu units box**… creates copper atoms in the simulation box**

regioncu1 prism 30 50 40 60 0 50 20 0 0 units box**defines a geometric region of V-notch**

group crystal region cu1

delete_atoms group crystal**… creates square-notch in the simulation box**

timestep 0.002**…… sets the timestep for subsequent simulations**

pair_styleeam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu**……specifies the potential file used**

 # Energy Minimization

#minimize 1.0e-7 1.0e-8 1000 1000

thermo 100 **computes and prints thermodynamic**

thermo_style custom step temp vol press etotal **specifies content of thermodynamic**

data to be printed in screen &

computemyRDF all rdf 1000

fix 11 all ave/time 10 1 10 c_myRDF file cu_melt_new.rdf mode vector

dump 1 all atom 10 Cu_crystal_melt_3d_s_dump_new.lammpstrj

..… dumps a snapshot of atom quantities every 10 time steps

to the specified file

dump_modify 1 scale no**…** **modifies parameters of previously defined dump command.**

A value of scale 'no' means atom coordinates are written in absolute distance units.

log logCu_crystal_melt_3d_s_new.data

… **closes the current log file, opens a new log file, and begins logging information to it**

velocity all create 300 873847 rot yes mom yes distGaussian **…** **sets the velocity of a**

group of atoms

#fixes

fix 1 all npt temp 100 100 0.1 iso 0 0 0.1 **temp and pressure conserved**

run 1000**…** **program is run for 1000 iterations**

unfix 1 **…** **deletes the previously defined fix 1**

3.5. Tensile Test:

It is speculated for any MD simulation study that an energy minimization of the system is necessary before performing the actual simulation studies. Through repetitive adjustment of atom coordinates, the configuration attains a position of minimum local potential energy. The configuration used for tensile testing was therefore equilibrated at room temperature using the method described above. The tensile test was then carried out at five different temperatures viz.
100 K, 200 K, 300K, 400K and 500 K with the parameters as mentioned in Table 1. The strain in the y direction was calculated using the following equation:

$$e = \text{loading rate} * \text{time} \qquad (3.4)$$

Where time = time step * step number (time step = 0.001 ps)
Loading rate = 0.1/ps

To understand the effect of notch geometry, simulations were carried out with similar box dimensions [Table 1] and the typical outcome obtained was plotted in the form of stress-strain curves.

3.5.1. Input file for tensile testing of a previously equilibrated crystal:

 # 3d tensile simulation JP4review

```
units           metal
boundary        p pp
atom_style      atomic
echo        both
read_data       Test.dat reads the data file containing the  atom positions of the equilibrated crystal in the specified file
timestep        0.001
pair_style      eam/alloy
pair_coeff          * * Cu_zhou.eam.alloy Cu

# Energy Minimization
#minimize           1.0e-5 1.0e-10 10000 100000
dump                1 all atom 100 dump.Test_40%strain.lammpstrj
log log5050_Test_40%strain.dat
```

initial velocities

velocity all create 300 482748 rot yes mom yes distgaussian

fix 1 all deform 1 y erate 1.0**….□strain rate of 0.1 sec^{-1} is applied in y direction**

fix 2 all npt temp 100.0 100.0 10.0 x 0 0 10.0 z 0 0 10.0 dilate all**…□all atoms rescaled to new positions while temp and pressure is conserved**

fix 3 all temp/rescale 10 100 100 0.05 1.0□**Resets the temp of atoms to 100K by rescaling velocities after every 10 steps**

compute 11 all rdf 100

fix 4 all ave/time 100 1 100 c_11 file rdf_Test_40%strain.rdf mode vector

compute 1 all stress/atom **…□ computes the symmetric per-atom stress tensor for each atom in a group.**

compute 2 all temp**… □ computes the temp of a group of atoms**

dump 2 all custom 1000 dump.stress_atom_Test_40%strain type x y z c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_1[6]□**dumps atom type; x,y,z coordinates; 6 stress tensors computed in 1 to an array of 6 elements**

compute 3 all reduce sum c_1[2]□**reduces vector quantities of all stress tensors in y-direction and adds all the quantities to a single**

variable stress equal c_3/(3*40000)□**assigns a value to the variable name stress**

variablestress_GPa equal v_stress/10000□**converts the stress calculated to GPa**

variablestress_MPa equal v_stress_GPa*10000

variable tmp equal ly

variable lo equal ${tmp}

variable strain equal (ly-v_lo)/v_lo

variable p equal -pyy/10000□**assign a value to the variable name strain**

thermo 10

thermo_style custom step temp press voletotal c_2 v_stressv_stress_GPav_stress_MPav_strain

run 4000**…** □ **number of iterations is given so as to give 40% strain to the material**

3.5.2.The Ductile fracture in Nanoscale Copper through Tensile Simulation code

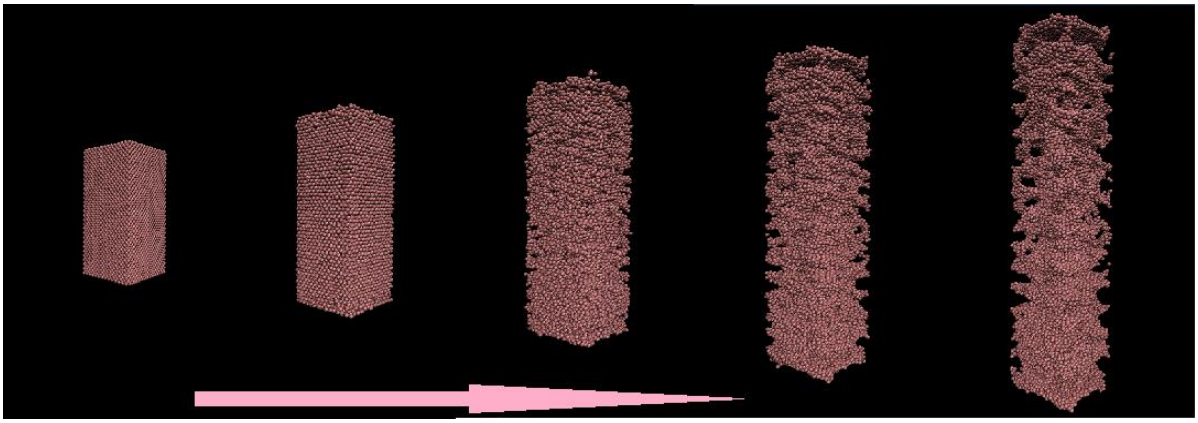


Fig-3.b.i: VMD snapshot of tensile testing of unnotched specimen during simulation

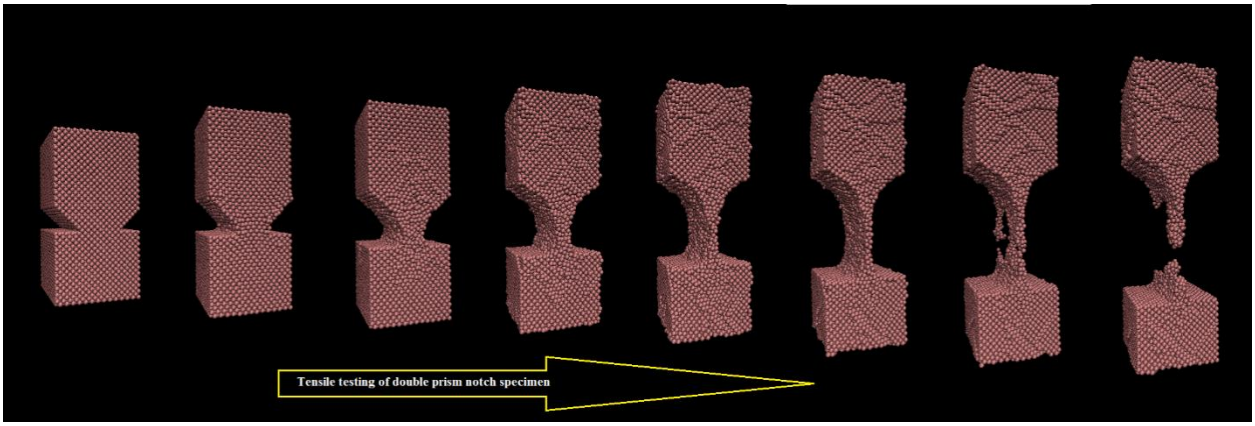


Fig-3.b.ii: VMD snapshot of tensile testing of Double V-notched specimen during simulation

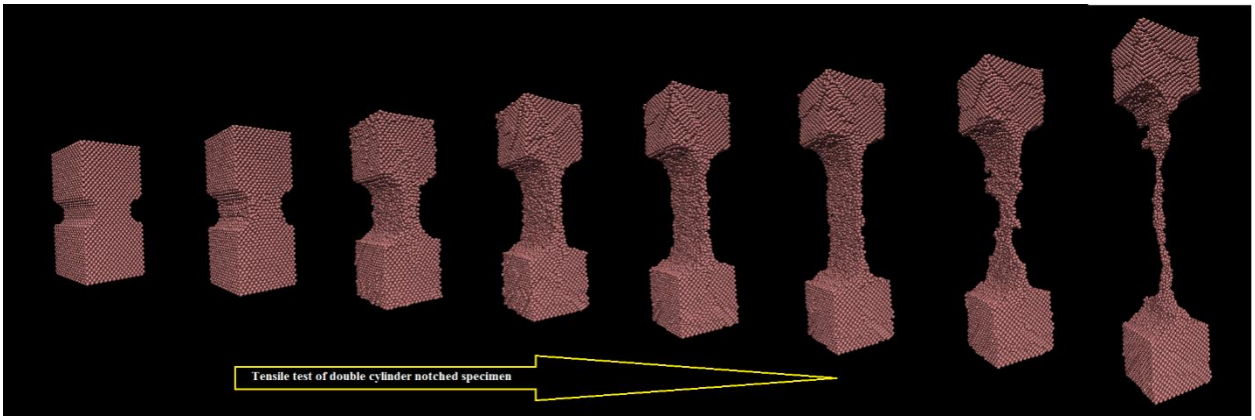


Fig-3.b.iii: VMD snapshot of tensile testing of Double cylindrical notched specimen during simulation

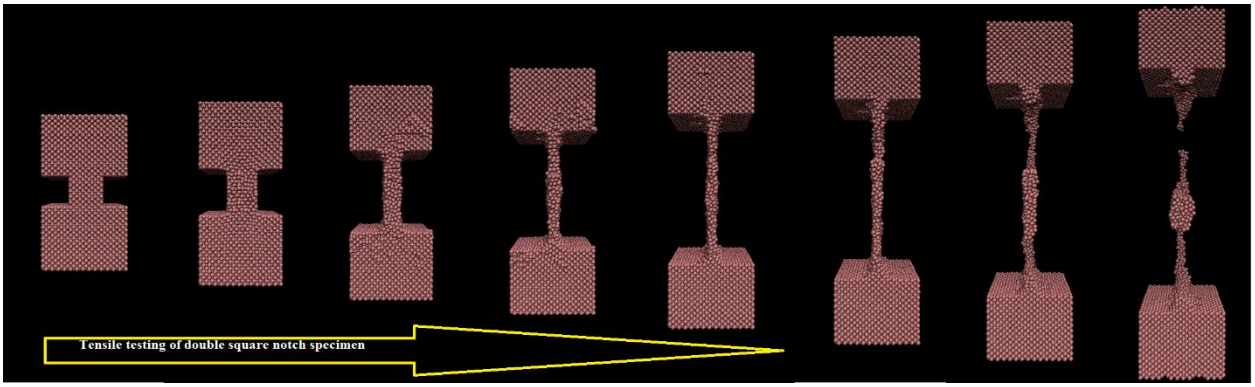


Fig-3.b.iv: VMD snapshot of tensile testing of Double square notched specimen during simulation

3.6. Compression Test:

In this experiment we also test the hardness of the materials at -0.1 strain rate with similar temperature (i.e. Room temperature) . Unlike the tensile testing here we get deformation of the Copper at a very low strain rate. The codes for compression in MD Simulations is same as Tensile simulation but here only the strain rate is negative and run time is much smaller in compare to tensile simulation**.**

3.6.1. Input file for compression testing of equilibrated crystal:

 # 3d compression simulation JP4review

units metal
boundary p pp
atom_style atomic
echo both
read_data Test.dat **reads the data file containing the atom positions of the equilibrated crystal in the specified file**

timestep 0.001

pair_style eam/alloy

pair_coeff * * Cu_zhou.eam.alloy Cu

Energy Minimization

#minimize 1.0e-5 1.0e-10 10000 100000

dump 1 all atom 100 dump.Test_40%strain.lammpstrj

log log5050_Test_40%strain.dat

initial velocities

velocity all create 300 482748 rot yes mom yes distgaussian

fix 1 all deform 1 y erate-1.0**….□strain rate of -0.1 sec^{-1} is applied in y direction**

fix 2 all npt temp 100.0 100.0 10.0 x 0 0 10.0 z 0 0 10.0 dilate all**…□all atoms rescaled to new positions while temp and pressure is conserved**

fix 3 all temp/rescale 10 100 100 0.05 1.0□**Resets the temp of atoms to 100K by rescaling velocities after every 10 steps**

compute 11 all rdf 100

fix 4 all ave/time 100 1 100 c_11 file rdf_Test_40%strain.rdf mode vector

compute 1 all stress/atom **…□ computes the symmetric per-atom stress tensor for each atom in a group.**

compute 2 all temp**… □ computes the temp of a group of atoms**

dump 2 all custom 1000 dump.stress_atom_Test_40%strain type x y z c_1[1] c_1[2] c_1[3] c_1[4] c_1[5] c_1[6]□**dumps atom type; x,y,z coordinates; 6 stress tensors computed in 1 to an array of 6 elements**

compute 3 all reduce sum c_1[2]□**reduces vector quantities of all stress tensors in y-direction and adds all the quantities to a single**

variable stress equal c_3/(3*40000)□**assigns a value to the variable name stress**

variablestress_GPa equal v_stress/10000□**converts the stress calculated to GPa**

variablestress_MPa equal v_stress_GPa*10000

variable tmp equal ly

variable lo equal ${tmp}

variable strain equal (ly-v_lo)/v_lo

variable p equal -pyy/10000 **assign a value to the variable name strain**

thermo 10

thermo_style custom step temp press voletotal c_2 v_stressv_stress_GPav_stress_MPav_strain

run 4000… **number of iterations is given so as to give 40% strain to the material**

3.6.2.The Brittle fracture in Nanoscale Copper through Compression Simulation code

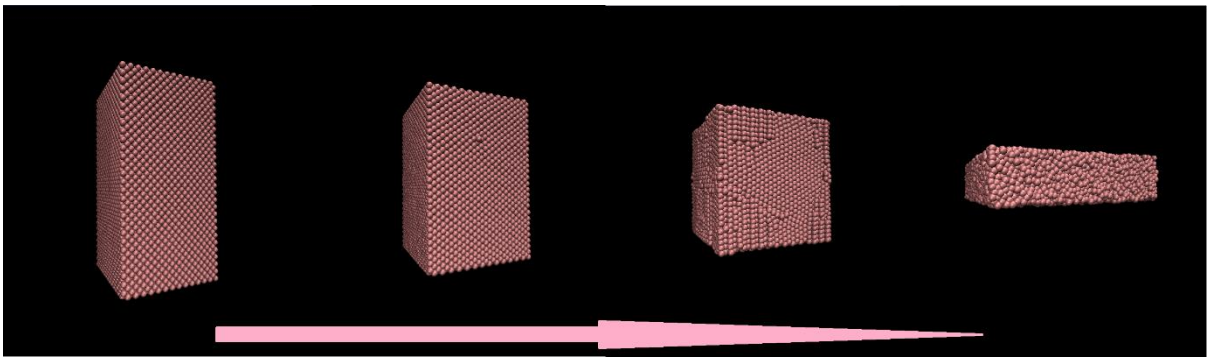


Fig. 3.c.i: VMD snapshot of Compression testing of unnotched specimen during simulation

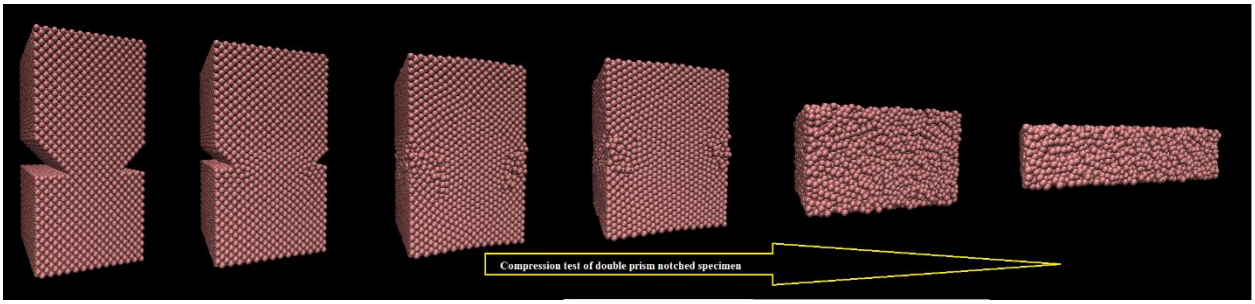


Fig. 3.c.ii: VMD snapshot of Compression testing of Double V-notched specimen during simulation

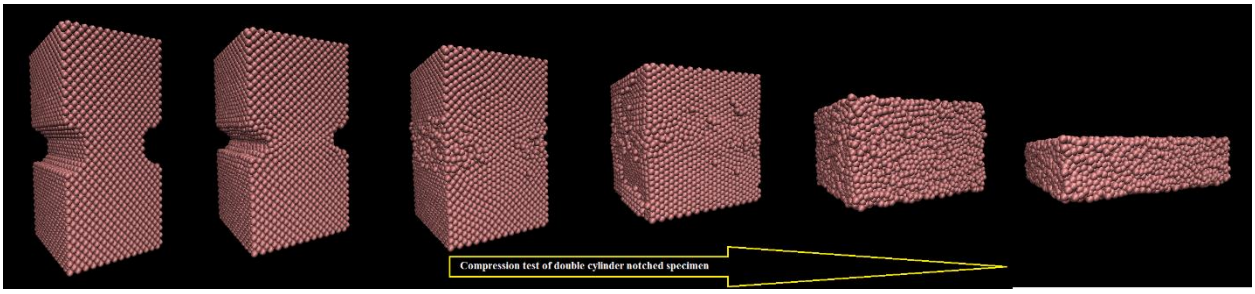


Fig. 3.c.iii: VMD snapshot of Compression testing of Double cylindrical notched specimen during simulation

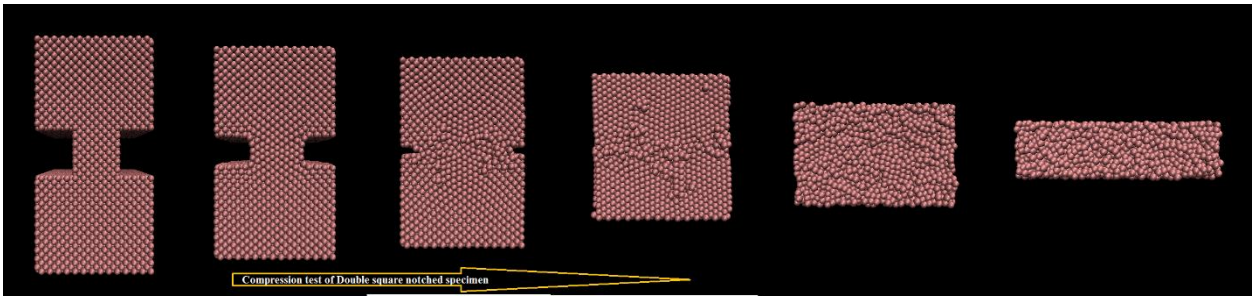


Fig. 3.c.iv VMD snapshot of Compression testing of square notched specimen during simulation

CHAPTER 4

RESULTS AND DISCUSSION

OUTLINE

- Tensile properties
    - Effect of temperature on tensile behaviour
    - Effect of notch design on tensile behaviour
- Compression properties
    - Effect of notch design on compression behaviour

RESULT AND DISCUSSION:

4.1Tensile Properties:

The primary aim of this investigation is to study the effect of various notch geometries (which is square notched, V- notched, cylindrical notched) on the tensile behaviour of nano-scale pure copper. Before conducting any experiment related to it, Molecular Dynamics simulations using LAMMPS were carried out to find tensile behaviour and hence UTS of the investigated material at various temperatures

4.1.1 Effect of temperature on tensile behaviour:

Simulations were carried out at various temperatures to study the effect of temperature on the tensile properties of nano-scale copper of various notch shape. The generated results from tensile simulations were observed and the data were plotted to generate the stress vs. strain curves of nano-scale copper at various temperatures (100K, 300K and 500K). Stress vs. strain curves are given in the below figures:

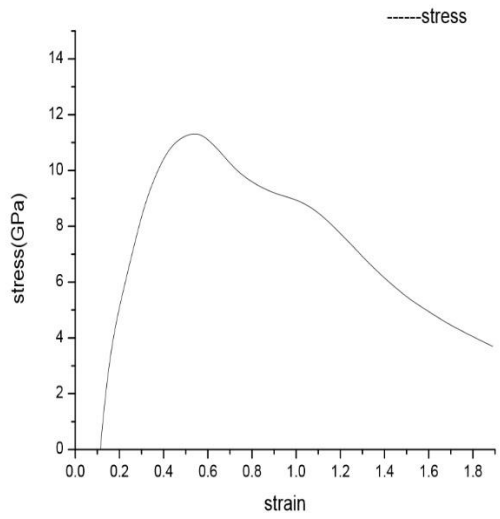


Fig.-4.a: Tensile stress vs strain at 100K in an unnotched specimen

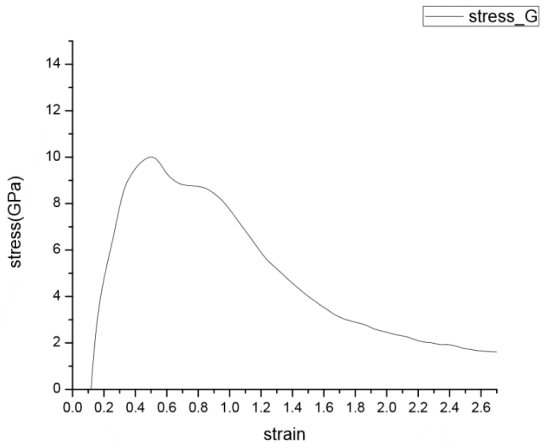


Fig.-4.b: Tensile stress vs strain at 300K in an unnotched specimen

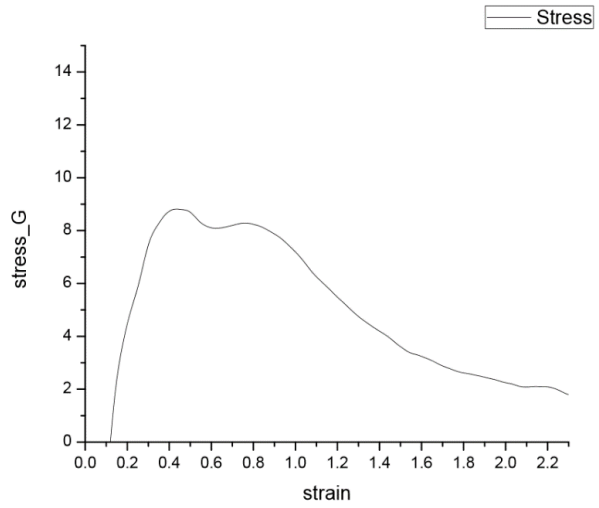


Fig.-4.c: Tensile stress vs strain at 500K in aunnotched specimen

This is well verified that strength of metallic materials decreases with increasing temperature.

From the simulation results on nano-scale copper, similar results has been obtained. The

Stress- strain curves at 100 K, 300 K and 500 K when plotted in a single graph clearly indicate the effect of temperature as illustrated in Fig. 4.6.

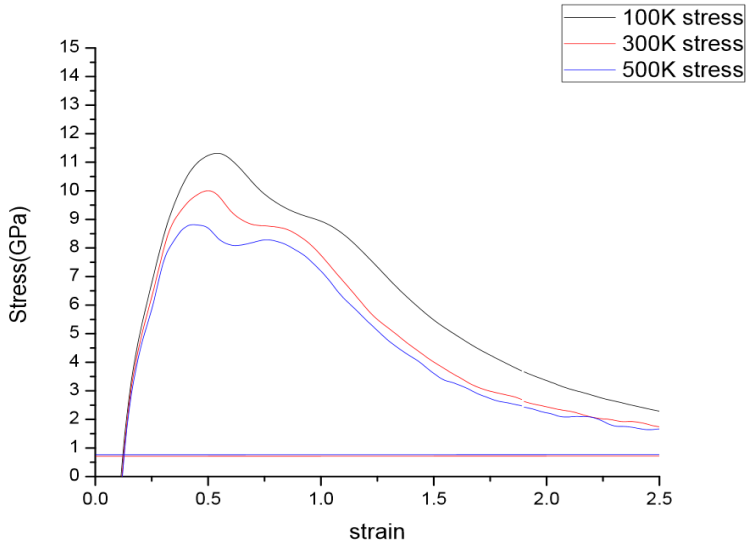


Fig.-4.d: Relationship between Tensile stress vs strain at various temperatures in a unnotched specimen

As the experiment procedure is shown in above, similar procedure is followed for different notch geometries and analyzed the effect of temperature on the tensile stress.

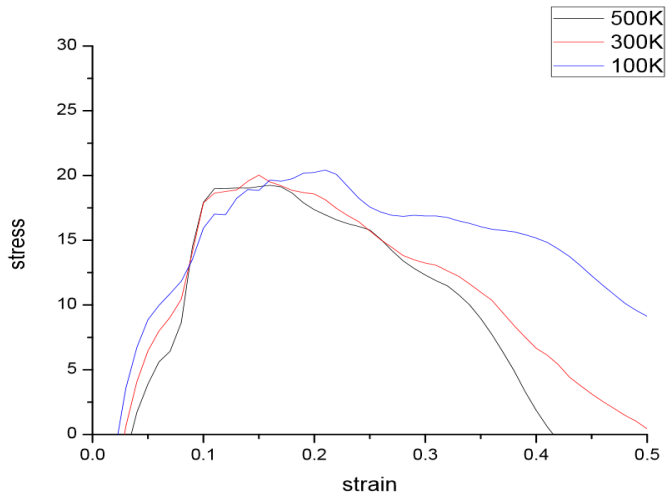


Fig.-4.e: Relationship between Tensile stress vs strain at various temperatures in a Double square notched specimen

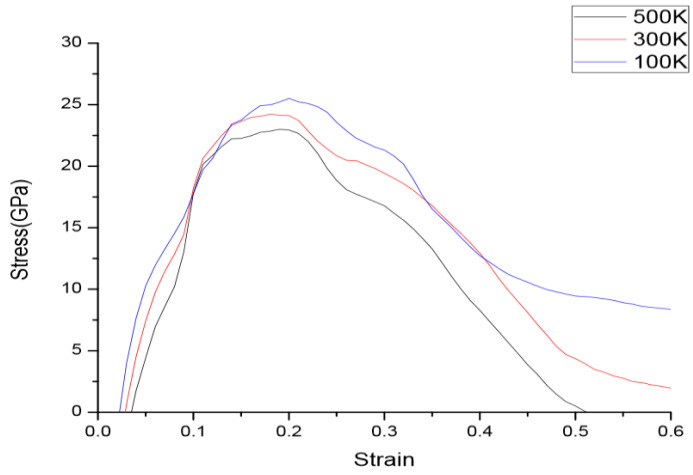


Fig.-4.f: Relationship between Tensile stress vs strain at various temperatures in a cylindrical notched specimen

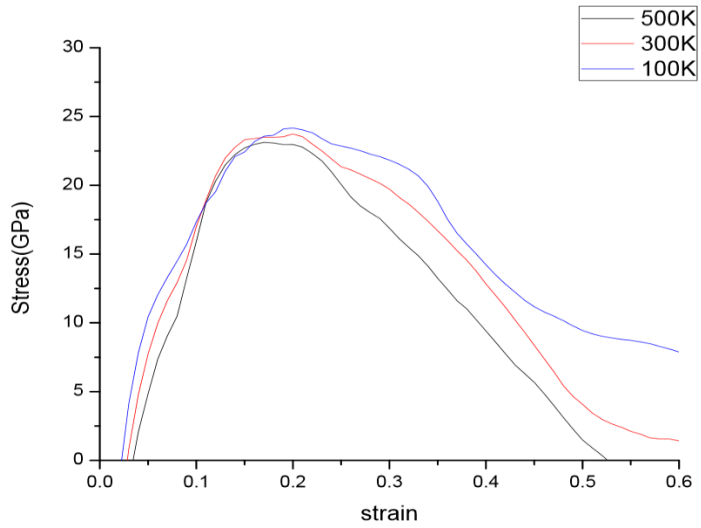


Fig.-4.g: Relationship between Tensile stress vs strain at various temperatures in a V- notched specimen

From the figure above we can assume that with increase in temperature, the stress vs. strain curves decreases, as we have expected. We know that flow stress drops down at higher temperatures; similar aspects can be observed by the current set of simulation studies.

The interatomic distance decreases because of increase in temperature. So the Ultimate Tensile Strength drops down on increasing temperature. The Ultimate Tensile Strength of a specimen is more temperature dependent than YS in the plastic region. After yielding the factors which effect UTS or interatomic distance will be less as other factors in plastic region like dislocation, voids etc. may come along with higher

interatomic distance Also it can be observed that with increase in temperature elongation and ductility will be more.

4.1.2. Effect of notch design on tensile behaviour

It can be predicted that based on number of atoms present in a cluster of atoms the properties of nano-scale materials should vary. This can be shown as the variations in notch geometry design. ; To study the effect of notch geometry on the tensile properties of nano-scale copper with notch and without notch Simulations were carried out at different temperatures. The output results from the tensile simulations were examined and the data were plotted to generate the stress vs. strain curves of nano-scale copper at multiple notch geometries at a specific temperature and study the effect of different notch shape on tensile character of nano-scale copper. Stress vs. strain curves were given in the below figures:

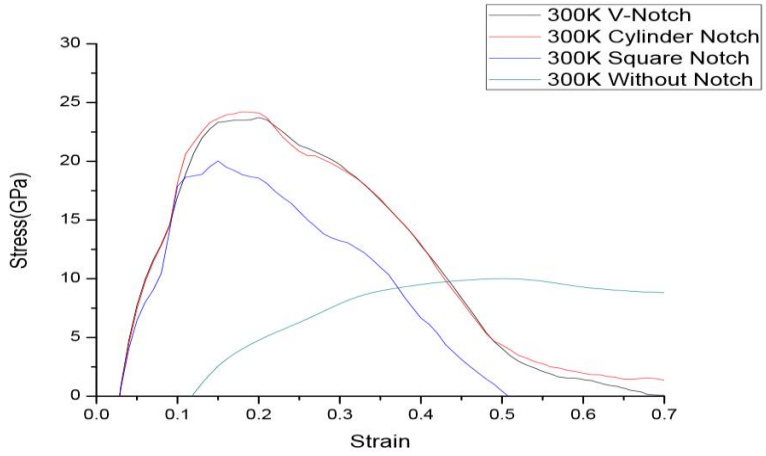


Fig.-4.h: Relationship between Tensile stress vs strain at various notch geometries at 300K

Similarly we can verify the effect of notch geometries on tensile stress at various temperature.

From the fig.-4.h we can see unnotched specimen's Ultimate Tensile Strength <cylindrical notched specimen's Ultimate Tensile Strength < prism notched specimen's Ultimate Tensile Strength < square notched specimen's Ultimate Tensile Strength

Significant effect of the notch is to create stress tri-axiality at the notch. It creates a local stress peak at the root of the notch with the introduction of notch. The tendency to increase tensile strength in presence of a tri-axial stress field is called notch sensitivity .With the introduction of notch there comes a plastic constraint factor. Due to this plastic constraint factor tensile strength will be greater than an unnotched specimen. Because of the presence of four sharp corner in double square notch, the stress triaxiality and plastic constraint factor will be greater as compared to other notched specimen. So Ultimate Tensile Strength will be greater in this case. Moreover it also can be observed that during tensile loading elongation and ductility reduces in presence of notch.

In below table, from the above stress- strain plots the value of Ultimate Tensile Strength, , , Yield Strength, %total elongation at various notch geometry, % uniform elongation and at various temperature were calculated

Temp.	Material Type.	UTS(GPa)	YS(GPa)	%Uniform elongation	%Total elongation
100K	Without Notch	11.326	4.23	0.535	1.89
100K	Double Square Notch	20.41	8.78	0.209	1.40
100K	Double Cylindrical Notch	25.42	24.607	0.212	2.003
100K	Double V-Notch	26.7	13.09	0.225	2.006
300K	Without Notch	10.00	3.34	0.498	2.69
300K	Double Square Notch	25.11	4.53	0.204	1.99
300K	Double Cylindrical Notch	24.29	23.22	0.192	1.189
300K	Double V-Notch	25.62	23.39	0.21	1.381
500K	Without Notch	8.819	2.802	0.429	2.29
500K	Double Square Notch	19.24	18.99	0.212	1.998
500K	Double Cylindrical Notch	22.92	21.42	0.183	1.219
500K	Double V-Notch	24.11	22.24	0.2	1.382

Table-4.1: Calculation of UTS, yield strength, % uniform elongation, % total elongation with different notch geometry at various temperature

4.2 COMPRESSION PROPERTIES:

4.2.1.. Effect of notch design on compression behaviour:

This is possibly can be interpreted as the notch geometry design variations. ; At various temperatures Simulations were carried out to study the effect of Double notch with various geometry on the compression behaviour of nano-scale copper with various notched and without notched specimen. From the generated results the tensile simulations were examined and the data were plotted to get the stress-strain curves of nano-scale copper at various double notch geometries at a particular temperature and study the effect of different notch geometries on compression behaviour of nano-scale copper. Stress vs. strain curves were illustrated in the figures below

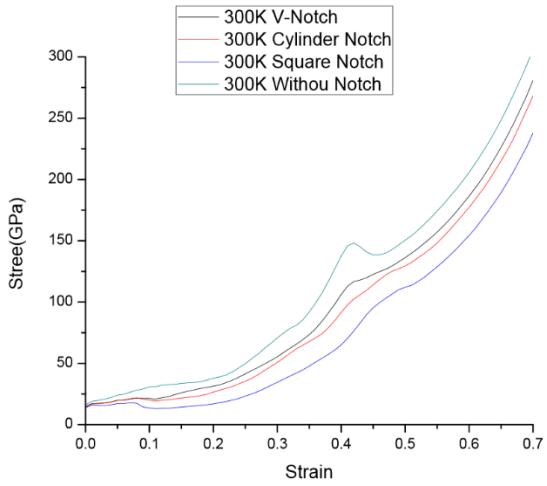


Fig.-4.i: Relationship between compression stress vs strain at various notch geometries at 300K

Similarly we can verify the effect of notch geometries on compression stress at various temperature.

From the fig.-4.i we can see unnotched specimen's compression stress > prism notched specimen's compression stress > square notched specimen's compression stress > cylindrical notched specimen's compression stress.

During the compression test, as copper is ductile material so after a short elongation the specimen is captured out of the box. The compression test is easy to measure for brittle material like ceramic but due to crack propagation and fracture ductile material it is difficult after a certain elongation point. In the cylindrical notched specimen the number of atoms present is least among the other notched specimen. Hence the fracture will be less required for compression stress.

CHAPTER 5

CONCLUSIONS AND SCOPE OF FUTURE WORK

OUTLINE

- CONCLUSION
- SCOPE OF FUTURE WORK

5.1 Conclusions:

We have studied the influence of temperature and different types of notch geometry on the tensile and compression behaviour of nano-scale copper by using molecular dynamics simulation. According to simulation results, the following conclusions can be assumed:

a) The ultimate tensile strength (UTS) of nano-scale copper is found to decrease from 11.326 GPa to 8.819 GPa when the temperature increase from 100K to 300K in un-notched condition. Similarly decrease in UTS is found for all double notched specimen.

b) It is shown that the tensile strength and ductility is greatly dependent on the geometry of the notches. The square notch is having maximum detrimental effect.

c) In a similar manner to the tensile simulations, compression strength of the specimen decreases with the influence of notch shape. It is found that the cylindrical notch is having maximum detrimental effect.

d) As one can assume the ductility of all notch specimen boxes reduces as compared to that in un-notched conditions. The reduction in ductility occurs due to development of plastic constraint factor in the notched specimens.

MD simulations is a good investigation than those obtained from laboratory experiments. Thus, it can be suggested that MD simulations can predict the tensile and compression behaviour of copper.

5.2. Scope of Future work:

In this investigation, tensile and compression behaviour of nano-scale pure copper has been studied. Careful analyses of the outcomes of this investigation may lead to the following scopes of further studies:

(i) To study the long duration effect of temperature on the compression behaviour of nano-scale copper, various temperatures simulations on compression can be conducted.

(ii) Simulations on tensile tests can be conducted to study the effect of strain rate and box dimension on tensile behaviour of the materials,.

(iii) Similar the tensile and compression behaviour of various other FCC materials like nickel, aluminium can be observed by conducting the simulation. The results we get from these simulations can be used for further analysis and understanding the variation in their tensile and compression behaviour.

(iv) Similar investigation can be done for multiple notches and various notch locations like double notch present in one end or double notches from both sides etc.

REFERENCE:

[1]. H. Inoue, Y. Akahoshi, S. Harada, Mater. Sci. Res. Int. 1 (1995) 95– 99.

[2]. B. Bhushan (Ed.), Handbook of Micro/Nano Tribology, CRC Press, New York, 1995.

[3]. N. Miyazaki, Y. Shiozaki, JSME Int. J. Ser. A 39 (1996) 606.

[4]. R.E. Miller, V.B. Shenoy, Nanotechnology 11 (2000) 139.

[5]. P. Heino, H. Hakkinen, K. Kaski, Phys. Rev. B 58 (1998) 641.

[6]. G. Z. Kang, Y.G. Li, J. Zhang, Y.F. Sun, Q. Gao, Theor. Appl. Fract. Mech. 43 (2005) 199–209.

[7]. L.J. Chen, Z.G. Wang, G. Yao, J.F. Tian, Int. J. Fatigue 21(1999) 791

[8]. B. Li, L. Ries, M.de Freitas, Int. J. Fatigue 28 (2006) 451–458.

[9]. L. Ristic (Ed.), Sensor Technology and Devices, ArtechHiuse, Boston, 1994.

[10]. U.S. National Report, WTEC Panel Report on Nanostructure Science and Technology R&D Status and Trends in

[11]. T. Aya, T. Nakayama, JSME Int. J. Ser. A 40 (1997) 343.

[12]. C.K. Hu, B. Luther, F.B. Kaufman, J. Hummel, C. Uzoh, D.J. Pearson, Thin Solid Films 262 (1995) 84.

[13]. J. Schiotz, T. Vegge, F.D. Di Tolla, K.W. Jacobsen, Phys. Rev. B 60 (1999) 11971

[14]. ASTM, Philadelphia, PA. E8M-08, (2008), Stand. T. M. for Ten. T. of M M, Annual Book of ASTM Standards, 03.01, E8M-08, (2008)

[15]. G. E. Dieter, Mechanical Metallurgy, SI metric edition, McGraw-Hill Book

Company, Singapore (1987),